

High-temperature superfluidity of fermionic atoms in optical lattices

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The experimental realizations of degenerate Bose [1] and Fermi [2–5] atomic samples have stimulated a new wave of studies of quantum many-body systems in the dilute and weakly interacting regime. The intriguing prospective of extending these studies into the domain of strongly correlated phenomena is hindered by the apparent relative weakness of atomic interactions. The effects due to interactions can, however, be enhanced if the atoms are confined in optical potentials created by standing light waves [6–8]. The present Letter shows that these techniques, when applied to ensembles of cold fermionic atoms, can be used to dramatically increase the transition temperature to a superfluid state and thus make it readily observable under current experimental conditions. Depending upon carefully controlled parameters, a transition to a superfluid state of Cooper pairs [9], antiferromagnetic states [10] or more exotic d-wave pairing states [11] can be induced and probed. The results of proposed experiments can provide a critical insight into the origin of high-temperature superconductivity in cuprates [12].

An active search is now under way to implement a BCS transition of degenerate fermionic gases to a superfluid state analogous to superconductivity [13,14]. However, in free space or weakly confining atom traps the transition temperature to the superfluid state scales exponentially with interaction strength, $k_B T_c^{\text{free}} \approx 0.3 E_F^{\text{free}} \exp[-\pi/(2k_F |a_s|)]$, with E_F^{free} the Fermi energy. For a dilute atomic gas the product of Fermi momentum and scattering length $k_F |a_s| \ll 1$, which makes the transition temperature exceedingly low.

Atoms in potentials created by standing light waves (optical lattices) tend to localize near potential nodes thereby increasing the strength of effective interactions, whereas the kinetic energy provided by tunneling between the different sites can be strongly suppressed [6]. Very recently, fascinating experiments involving bosonic atoms in optical lattices [7] revealed a quantum phase transition from a superfluid to Mott insulating state [6,15]. Fermionic atoms confined in an optical lattice can undergo a phase transition to a superfluid state at a temperature that exceeds that of weakly confined atoms by several orders of magnitude. Attractive atomic interactions result in an s-wave pairing in which case fermionic

atoms can undergo a BCS-type transition. In what perhaps is the even more intriguing prospective, fermionic atoms with repulsive interactions correspond to an experimental realization of a Hubbard model that is widely discussed for strongly correlated electron systems such as high- T_c cuprates [16]. In particular, d-wave superconducting states have been conjectured to exist in such systems, but so far this conjecture eluded rigorous confirmation. We show that atomic systems with carefully controllable parameters and a variety of precise tools to detect the resulting phases can be used to provide a critical insight into this outstanding problem. In essence, this approach can be viewed as an implementation of the pioneering ideas due to Feynman [17] for simulations of one quantum system by another.

Consider an ensemble of fermionic atoms illuminated by several orthogonal, standing wave laser fields tuned far from atomic resonance. These fields produce a periodic potential for atomic motion in two (or three) dimensions of the form $V(x) = V_0 \sum_{i=1}^{2(3)} \cos^2(kx_i)$ with k the wave-vector of the light. The potential depth V_0 is typically expressed in the units of the atomic recoil energy $E_R = \hbar^2 k^2 / 2m$. We will be interested in the situation in which there is roughly one atom per lattice site. Such atomic densities correspond to free-space Fermi energies on the order of $E_F^{\text{free}} = (3/\pi)^{2/3} E_R$. At the same time the atoms can tunnel from one site to another. We assume that two kinds of atoms are present, differing by angular momentum or generalized spin ($\sigma = \{\uparrow, \downarrow\}$). For sufficiently low temperatures the atoms will be confined to the lowest Bloch band, and the system can be described by a Hubbard Hamiltonian [6,16]

$$H = -t \sum_{\{i,j\},\sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow},$$

where $c_{i,\sigma}$ are fermionic annihilation operators for localized atom states of spin σ on site i , $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$. We assume that the average occupation numbers $\langle n_{i,\uparrow;\downarrow} \rangle \leq 1$. The parameter t corresponds to the tunneling matrix element between adjacent sites, $t = E_R (2/\sqrt{\pi}) \xi^3 \exp(-2\xi^2)$, and the parameter $U = E_R a_s k \sqrt{8/\pi} \xi^3$ characterizes the strength of the on-site interaction with $\xi = (V_0/E_R)^{1/4}$. The sign of the scattering length a_s determines the nature of atomic interactions: negative a_s corresponds to attraction between atoms, whereas positive a_s corresponds to repulsion. For

example, in the case of Li^6 [3,4] both cases can be realized depending on the particular electronic states that are being trapped in a lattice.

Consider first the situation corresponding to negative U . The effect of the lattice on the superfluid transition can be best understood starting from the limit of large tunneling $t \gg |U|$. Here, similar to the free-space transition, the interaction strength is much weaker than the kinetic energy and the ground state of the system is then given by a “standard” BCS wave function, with an energy gap and transition temperature T_c that depend upon t and u [18]. For the lattice with filling fraction near unity ($\langle n_\uparrow \rangle + \langle n_\downarrow \rangle \sim 1$) the Fermi energy is on the order of t , the density of states scales as N/t (with N being the total number of lattice sites) and the average two-atom interaction strength as U/N . Standard BCS theory can be applied to predict a critical temperature T_c that for a 3-D situation scales as $k_B T_c \approx 6t \exp(-7t/|U|)$ [18]. An increase in the depth of the optical potential results in stronger atom localization and hence an increased interaction strength U . At the same time, the tunneling t becomes weaker. The combined effect of these two factors is a dramatic increase in T_c due the exponential factor that competes with a very modest linear reduction due to a decreased Fermi energy.

As the tunneling becomes comparable to the on-site interaction, the BCS picture is no longer valid. Due to strong attraction, atoms form pairs within single lattice sites. The entire system can then be considered as an ensemble of composite bosons. They can tunnel together at a rate $\sim t^2/|U|$, by virtual transitions via intermediate singly occupied states. In this regime non-ordered pairs exist at high temperatures, whereas the superfluid state - a condensate of composite bosons - appears below $k_B T_c \sim t^2/|U|$. Clearly, in this limit the increase in the potential depth will lead to a reduced mobility of pairs and hence a decrease in T_c . The maximal critical temperature T_c^{max} is achieved at the crossover between the two regimes, when interaction and tunneling are comparable (more precisely at $U \sim 10t$), which corresponds to a potential depth $\xi^2 \approx 1/2 \log[5\sqrt{2}/k|a_s|]$ and

$$k_B T_c^{\text{max}} \approx 0.3 E_F^{\text{free}} k|a_s|. \quad (1)$$

That is, the critical temperature for atomic fermions trapped in a lattice scales only *linearly* with the small parameter $k|a_s|$. This accurate result for the critical temperature is based on nonperturbative Monte-Carlo simulations of the fermionic Hubbard model [18].

Several specific approaches to achieve the superfluid state can be considered. For example, the optical potential can be adiabatically turned on, starting from a weakly confined Fermi-degenerate mixture of the two atomic states of appropriately chosen density. In this procedure the atomic quasi-momentum is approximately conserved but the band-structure associated with the periodic potential changes, resulting in a non-equilibrium

distribution, with an effective temperature T_f different from the initial T_{in} . The final temperature T_f can easily be estimated from the relation $\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} f(\epsilon_{\mathbf{k}}^0/T_{\text{in}}) = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} f(\epsilon_{\mathbf{k}}/T_f)$, where $f(x) = 1/(e^x + 1)$ is the Fermi-Dirac distribution function, $\epsilon_{\mathbf{k}}^0 = k^2/2m - \mu^0$ is the original dispersion of atoms in free space, and $\epsilon_{\mathbf{k}} = -2t(\cos(k_x a) + \cos(k_y a) + \cos(k_z a)) - \mu$ is the dispersion in a tight-binding model with $a = \pi/\lambda$ the lattice period. Two important processes determine T_f . First of all, the presence of the lattice makes the system anisotropic and hence changes the shape of the Fermi surface. This results in an effective heating of the system as V_0 increases from zero to about E_R . As V_0 is increased even further the shape of the Fermi surface remains approximately the same and only the Fermi velocity (or effective atomic mass) changes leading to a reduction of the effective temperature within the lowest Bloch band (see Fig. 1). This suggests that it is optimal to turn on a weak lattice potential while the fermionic sample is in contact with a cooling reservoir (e.g. atomic BEC). Although the resulting phase space density will not be significantly altered, this loading procedure will allow to avoid the heating which is present at the initial stages of creating an optical lattice. When $V_0 \sim E_R$ (point C in Fig. 1a) the system is decoupled from the reservoir and the lattice potential is increased until the transition to the superfluid phase is reached.

To control precisely the resulting quantum phase (especially in the situations described below) an accurate manipulation of the filling fraction may be important. This can be achieved, for example, if atoms with three internal states are used. If a dense, degenerate ensemble is prepared in a state that is not affected by the optical lattice, a laser driven Raman transition into a pair of trapped spin states can be used to produce exactly one atom (or its fraction) per each lattice site. The essential idea of this approach is that the energy shifts associated with atom interactions and the Pauli principle can be used to block the transitions into states with more than one atom per lattice site. In this case an effective $\nu\pi$ -pulse will result in a filling fraction of ν with an uncertainty that scales at most with the inverse size of the lattice.

Let us now consider the implications of these results in the light of present experimental possibilities. The relevant temperature calculated numerically for Li^6 [3] and K^{40} [2] atoms is shown in Fig. 1. In this figure we consider a Li^6 atomic sample of a very modest density corresponding to a unity filling in an optical lattice produced by CO_2 laser ($\lambda = 10\mu\text{m}$). For such densities, a dramatic increase in the critical temperature is possible. Note in particular that a phase transition can be achieved starting from an initial temperature of about $0.1 E_f^{\text{free}}$. The CO_2 lattice has the additional advantage of exceptionally long lifetimes, which should be sufficient to achieve the transition even for relatively low energy scales involved.

Another scenario is to trap Li atoms in an optical lattice created by a Nd:YAG laser $\lambda \sim 1.06\mu\text{m}$. Although in this case the densities of $10^{12} - 10^{13} \text{ cm}^{-3}$ will correspond to a filling fraction slightly less than unity, the resulting critical temperature can still be in the range of $0.1 E_F^{\text{free}}$. The inset shows a diagram for K^{40} atoms trapped in a similar lattice. As indicated by the two cases presented in Fig. 1 the transition to a superfluid state is expected to occur for the same initial temperature if cooling due to adiabatic switching on of the lattice is taken into account. Therefore, the value of the maximal initial temperature at which a phase transition can occur is *almost independent of the scattering length* and corresponds to about one tenth of the free space Fermi energy.

Before proceeding we point out that in contrast to the approaches that are based on increasing the scattering length or atom densities, which result in a very interesting regime of BCS-BEC crossover [19–21], an optical lattice does not lead to an enhancement of inelastic loss processes but rather their suppression, as no more than two atoms can ever occupy the same lattice site. We also note that this implies an extremely low spin flip rate between different atomic states, thereby allowing comparatively large magnetic fields to tune the scattering lengths without significantly perturbing the relative fractions of n_{\downarrow} and n_{\uparrow} . It is also important to point out that although the free-space ensembles at densities $n|a_s|^3 > 1$ can no longer be considered as weakly interacting gas [19,20], the Hubbard model nevertheless remains a valid description for the lattice case even in the regime of very strong confinement. Here corrections to the on-site interaction can be accurately derived from known molecular potentials. Finally we emphasize again, that in contrast to a weakly confined Fermi-gas, the critical temperature for the optical lattice filled with attractive atoms (Fig. 1) can be predicted very accurately even in the most interesting, intermediate, regime $t \sim |U|$, since the behaviour of the Hubbard model for this case is by now very well understood.

It is intriguing to consider possible extensions of the above ideas to a situation in which different atoms repel each other ($a_s > 0$). This is realized for $|\downarrow\rangle = |F = 9/2, m_F = 9/2\rangle$ and $|\uparrow\rangle = |F = 9/2, m_F = 7/2\rangle$ states of atomic K at zero magnetic field [2]. In this case it is energetically unfavorable for two atoms to be on the same lattice site. However, adjacent atoms can virtually tunnel to the same site. This process lowers the total energy of two atoms in adjacent wells, thereby creating effective hard-core attractive interactions of different spins. When the filling fraction of the lattice is close to one, this leads to a ground state in which adjacent sites are always occupied by atoms with alternating spins (see Fig. 2), i.e. an antiferromagnetic phase.

What happens when the filling fraction is smaller than one? This question lies at the heart of the present debates on the nature of high-temperature superconducting

cuprates. Clearly, a strong on-site repulsion makes it unfavorable for atoms to bind into the usual s-wave pairs, in which the probability to be at the center of orbit should be maximal. However, it has been conjectured [11] that anisotropic d-wave pairs can be formed, which can result in a d-wave superfluid phase capable of explaining many of the observed properties in cuprates.

d-wave Cooper pairs can be thought of as spin singlet angular momentum $l = 2$ Cooper pairs. In the absence of the lattice potential all five $l_z = \pm 2, \pm 1, 0$ components are degenerate. A cubic potential splits these states according to the representations of the cubic point group, and we find triply and doubly degenerate Cooper pairs [23]. When the symmetry of the crystal is lowered even more, as e.g. in a two dimensional lattice, the degeneracies between various Cooper pairs are removed further, and in the x, y directions the lowest energy Cooper pair is described by the momentum space wave function [24] $\Delta(\mathbf{p}) = \cos(p_x a) - \cos(p_y a)$. Although so far the existence of d-wave superconductivity in the repulsive Hubbard model eluded rigorous confirmation, we believe that these ideas can now be tested experimentally in ensembles of fermionic atoms. For example, Fig. 2 shows a phase diagram for the system of repulsive atoms in two dimensions [11] calculated using the FLEX approximation [25]. Although the resulting T_c is believed to be somewhat lower than in the s-wave case, this calculation suggests the existence of the d-wave phase for feasible atomic temperatures and densities.

We next consider several approaches that can be used to detect and accurately probe the resulting quantum phases. For example, interference of the atoms released from the lattice has been used to probe the superfluidity of bosons [7]. Due to the exclusion principle, identical fermions can never be in the same quantum state. This implies that in the degenerate regime atomic interference patterns due to each momentum state will be superimposed, resulting in real space interference peaks which reflect the shape of the Fermi surface. With the appearance of pairing, the atomic momentum in the pairs becomes on the order of Planck's constant divided by the size of the pair. As a result, the momentum distribution is no longer a sharp step function, which will be directly reflected in the interference pattern as shown in Fig. 3.

In order to directly detect superfluidity of the pairs, photoassociation spectroscopy [22] can be used. Weakly bound Cooper pairs can be converted into molecules by using a laser-induced transition into a bound molecular state. The interference pattern of the released bosonic molecules will then provide extremely sharp peaks due to the presence of a superfluid fraction, in direct analogy to ref. [7].

The spectrum of elementary excitations also provides an accurate probe for the nature of the quantum phase. It can be measured in a system of cold atoms by exciting the motional states of atoms using laser pulses. For

example, atoms can experience Bragg scattering off two non-collinear laser beams, provided that the frequency difference $\delta\omega$ of the lasers matches the resonance frequency of elementary excitation with momentum q determined by the angle between two lasers (Fig. 4) [26]. This technique provides a direct measurement of the density-density correlation function. By monitoring the number of Bragg-scattered atoms as a function of $\delta\omega$, the presence of a superfluid phase can be detected unambiguously: One observes a sharp peak due to a collective Bogoliubov mode, which is separated from a broad feature (corresponding to quasi-particle excitations) by an energy gap (see Fig. 4). In the normal state, on the other hand, the continuum excitations are gapless and the collective mode is not visible due to strong damping.

With this technique, it is also possible to detect d-wave superfluidity. For example, Fig. 5 shows the onset frequency of the quasiparticle continuum corresponding to the d-wave superfluid phase. A strong anisotropy, together with a vanishing gap for certain momenta can provide unambiguous evidence for the presence of such a phase.

It should be noted that in addition to the effects described here, a number of other intriguing avenues can be considered. Atomic systems make it possible to accurately probe the effects of dimensionality. Varying for example the depth of the trapping potential in one direction while keeping the other parameters fixed, it should be possible to observe a transition between a two-dimensional and a three-dimensional situation. One can also envision a situation in which more than two internal atomic states are trapped in the optical lattice. Such a system is expected to result in a variety of new quantum phases such as superconductivity based on quadruplets rather than pairs. Likewise, these systems might allow for accurate studies of the effect of dissipation and decoherence on macroscopic quantum phases. Another interesting phenomenon that may be studied by creating a system with unequal densities for the two spin states is the possibility of the Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) state [27,28] with a modulated superfluid order parameter.

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- [29] The authors gratefully acknowledge useful discussions with R. Hulet, J. Doyle and W. Ketterle. This work was supported by the NSF and the German Science Foundation (DFG). Work at the University of Innsbruck was supported by the Austrian Science Foundation. Correspondence should be addressed to E.D. (demler@physics.harvard.edu) and M.D.L. (lukin@physics.harvard.edu).

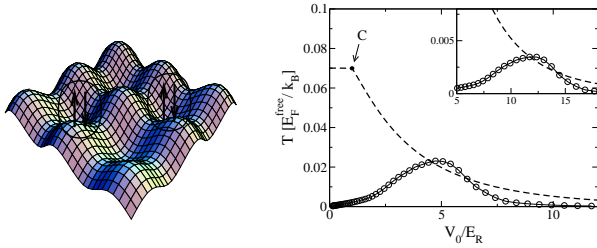


FIG. 1. Left: Attractive fermionic atoms in optical lattices can undergo pairing resulting in a BCS transition into a superfluid state. Right: Critical temperature for a transition of Li^6 atoms (circles) into the superfluid state as a function of the optical lattice depth in a three-dimensional CO_2 lattice. Li atoms in the states with different orientation of nuclear spin $|\downarrow\rangle = |F = 1/2, m_F = -1/2\rangle$ and $|\uparrow\rangle = |F = 1/2, m_F = 1/2\rangle$ are considered at a magnetic field of ~ 0.1 T which corresponds to a scattering length of $a_s \sim -2.5 \times 10^3 a_0$ in atomic units. The absolute energy scale is given by $t/\hbar \approx 0.5\text{kHz}$ at the phase transition. For the same values of the scattering lengths and densities the free-space BCS formula gives for the temperature of the superfluid transition $T_c^0 = 1.6 \times 10^{-12} E_F^{\text{free}}/k_B$ for Li^6 . The inset shows the analogous plot for K^{40} atoms in a Nd:YAG lattice at half filling. For K^{40} we took two states characterized by total angular momentum $|\downarrow\rangle = |F = 9/2, m_F = -9/2\rangle$ and $|\uparrow\rangle = |F = 9/2, m_F = -7/2\rangle$ at a magnetic field above a Feshbach resonance and choose $a_s \sim -2. \times 10^2 a_0$. As discussed in the text, turning on an optical lattice also changes the temperature of the system. It is most advantageous to turn on a weak lattice potential $V_0/E_R \sim 1$ while the atoms are cooled. The cooling is then switched off (point C in the figure) and the lattice depth is increased adiabatically, reducing the effective temperature (shown by the dashed line for an initial temperature $T_{\text{in}} = 0.07 E_F^{\text{free}}/k_B$).

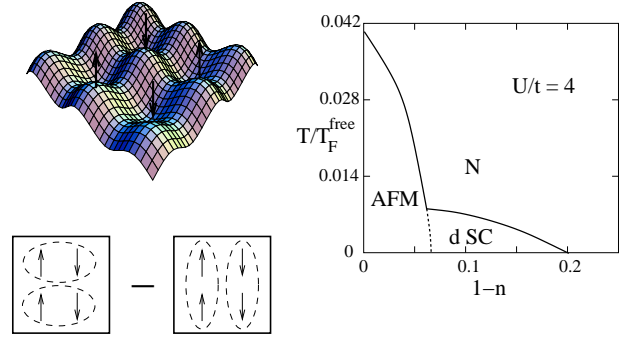


FIG. 2. In the case of repulsion it is energetically unfavorable for two atoms to be on the same lattice site. However, virtual tunneling creates effective hard-core attractive interactions of different spins on nearby sites. This may result either in antiferromagnetic (upper left) or d-wave superfluid phases, depending upon the filling fraction n . In three dimensions and at filling fraction $n = 1$ the maximum critical temperature for antiferromagnetic ordering is identical to the superfluid case, and of the order $0.1 E_F^{\text{free}}$. The d-wave symmetry of the superfluid is related to the “parent” insulating phase (see lower left). The phase diagram for repelling Li^6 atoms in a 2D lattice, calculated using the FLEX approximation, is shown on the right hand side. Adiabatic cooling due to switching on of the lattice has been taken into account. The situation we have in mind corresponds to a very large potential depth along one direction and an equal, finite depth along the other two directions. This results in a set of weakly coupled 2D lattices. Within each lattice tunneling is given by t . We note that the repulsive Hubbard model may also have phase separation for some filling factors, which corresponds to immiscibility of the two spin species of the atoms.

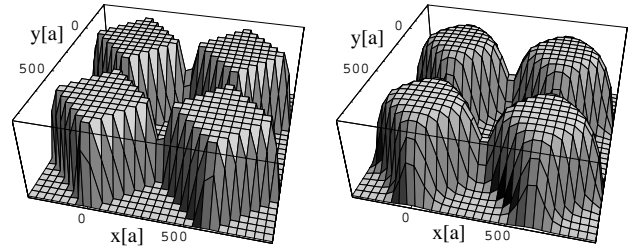


FIG. 3. Central part of the atomic interference pattern after a free expansion for $t = 500 \times (\hbar/E_R)$. We are considering a 10×10 optical lattice (a denotes the lattice constant). Left: normal state at half filling. The sharp edges of the interference peaks reflect the atomic momentum distribution: in the normal state the peaks will become sharper with decreasing temperature – a direct consequence of Fermi-statistics. Right: BCS state at half filling, with a gap $\Delta/t = 0.6$ corresponding to an interaction strength $U/t \approx -2.5$.

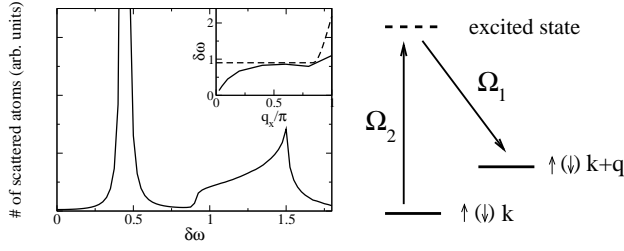


FIG. 4. Left: Bragg scattering of atoms off laser beams with frequency difference $\delta\omega$ and wave-vector difference $q_x = q_y = 0.1\pi$ for attractive fermions at filling $n = 0.6$ and $U/t = -2.5$, corresponding to an s-wave gap $\Delta/t \approx 0.45$. The spectrum consists of a sharp collective mode and a continuum at higher frequencies. The sharp resonance corresponds to long-wave coherent excitations of the condensate. The continuum arises due to the breaking of Cooper pairs, which results in quasiparticle excitations. In the inset we show the dispersion of the collective mode (solid line) and the onset frequency of the continuum (dashed line). Right: schematic picture of the two-photon process involved. Ω_1 and Ω_2 are the Rabi rates of the optical fields.

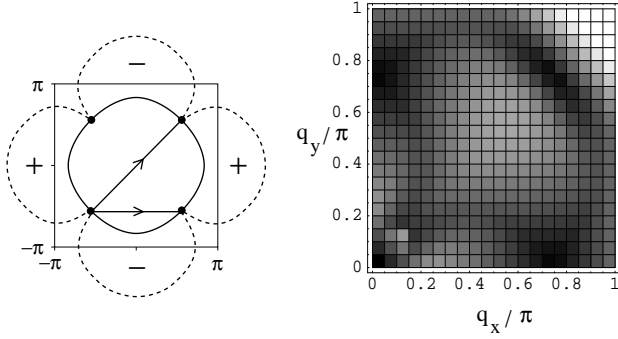


FIG. 5. Probing d-wave pairing at filling $n < 1$ via Bragg scattering. Left: schematic diagram of the Fermi surface (solid line) and the q -dependence of the Cooper pair wave function $\Delta(q_x, q_y)$ (dashed line). At the four nodal points shown by black dots, the wave function and the quasiparticle excitation energy vanishes. For the special wave vectors connecting these points, the density response is gapless (black spots in the right figure). Right: onset frequency $\omega_{\min}(q_x, q_y)$ of the quasiparticle continuum, dark regions corresponding to low frequencies (vanishing gap).